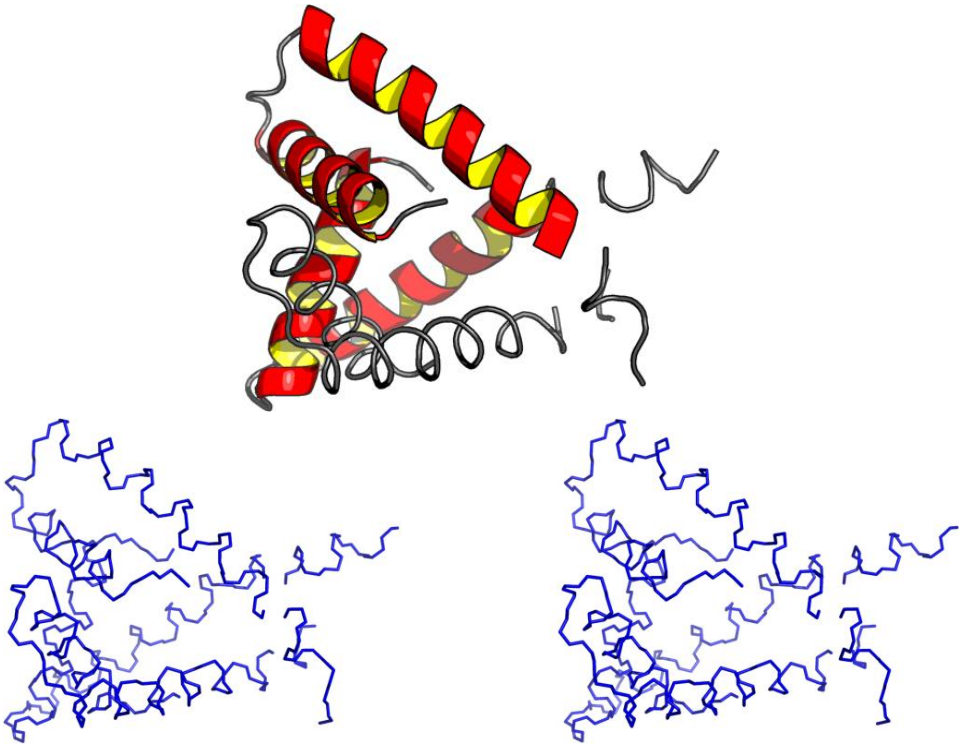
Structure Quality Analysis for NAME

Procheck analysis,RMSD calculation and structure superimposition are based on: all residues

NESG ID:	NAME
PDB ID:	
Deposition date:	
Common Name:	
Class:	
Length (a.a.):	154
Organism:	
SwissProt / TrEMBL ID:	
Oligomerization:	trimer
Molecular weight:	17334



Secondary Structure Elements:
Inter-chain break(s) between 52 & 63, 110 & 121
alpha helices: 4A-19A, 24A-48A, 4B-18B, 24B-39B, 42B-47B, 4C-19C, 24C-39C, 42C-46C
beta strands:

Resolution: 2.000 Å R-factor: 0.229 R-free: 0.262
Structure Factors deposited in the PDB? no

Ramachandran Plot Summary from Procheck

Most favoured regions	*Additionally allowed regions*	*Generously allowed regions*	*Disallowed regions*
94.6%	5.4%	0.0%	0.0%

Ramachandran Plot Summary from Richardson Lab's Molprobity

Most favoured regions	*Allowed regions*	*Disallowed regions*	View plot	View model summary
95.9%	3.4%	0.7%		

Global quality scores

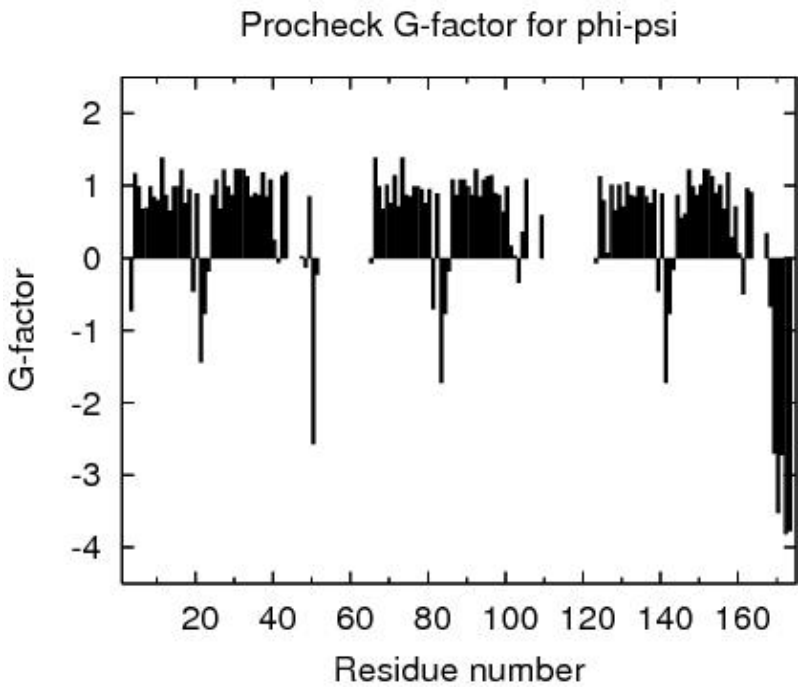
Program	*Verify3D*	*ProsaII (-ve)*	*Procheck (phi-psi)*	*Procheck (all)*	*MolProbity Clashscore*

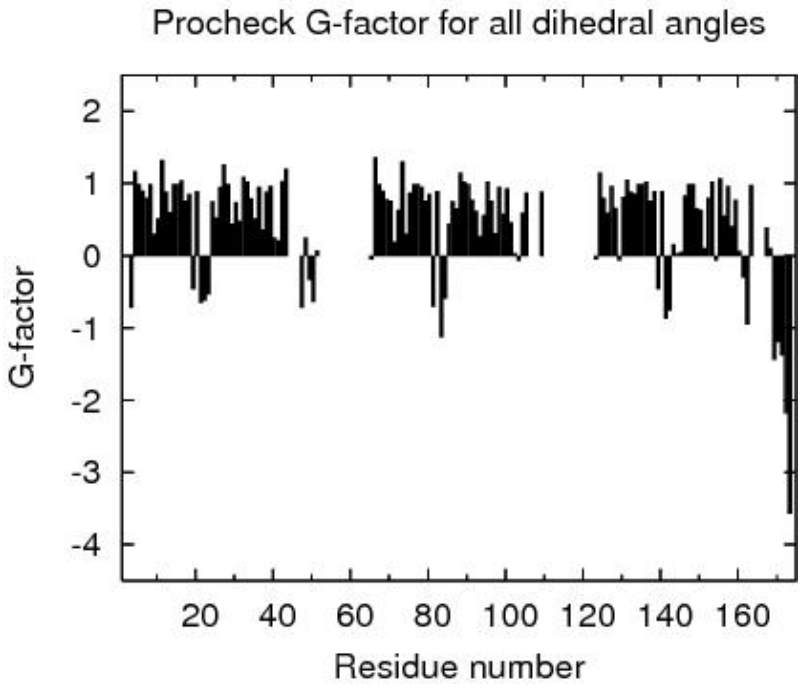
-Raw score	0.30	1.37	0.49	0.41	12.38
Z-score[1]	-2.57	2.98	2.24	2.42	-0.60

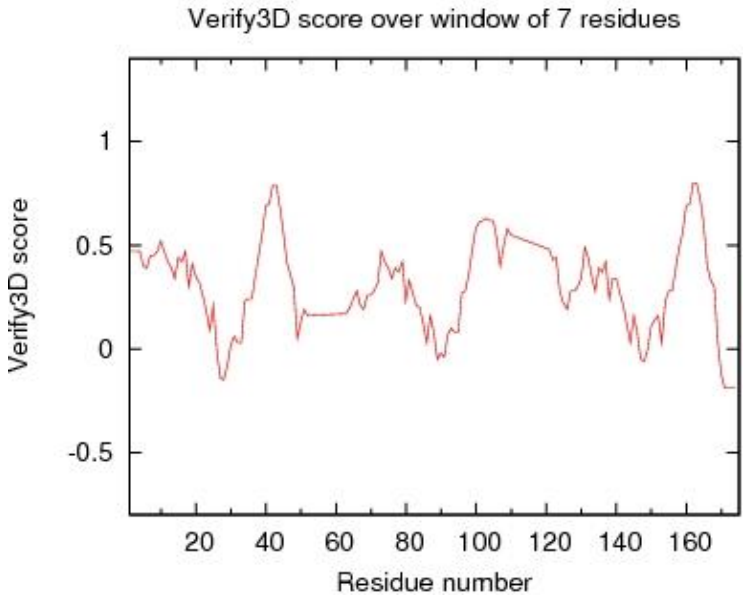
Close Contacts and Deviations from Ideal Geometry (from PDB validation software)

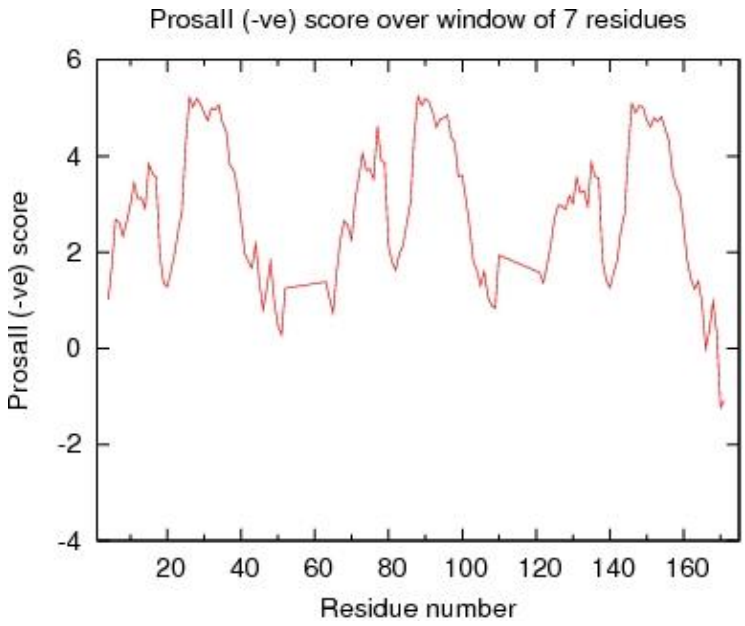
Number of close contacts (within 2.2 Å):	0
RMS deviation for bond angles:	0.8 °
RMS deviation for bond lengths:	0.005 Å

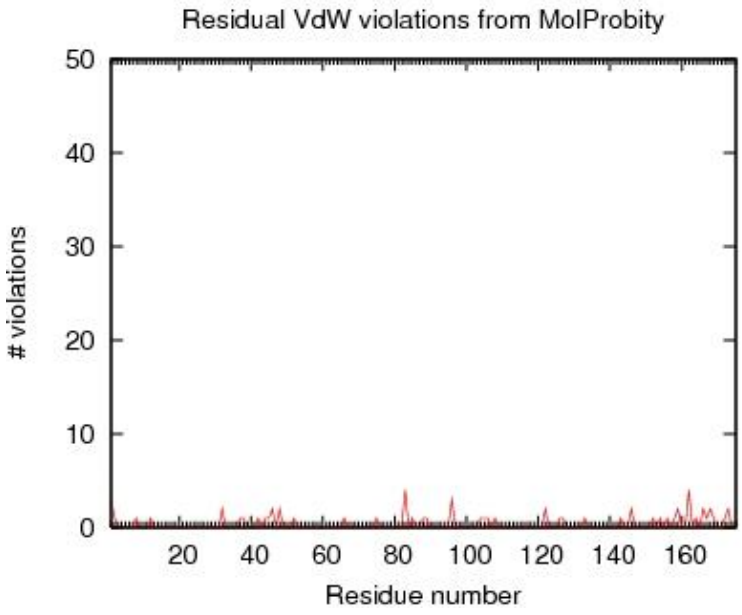
[1] With respect to mean and standard deviation for a set of 252 X-ray structures < 500 residues, of resolution <= 1.80 Å, R-factor <= 0.25 and R-free <= 0.28; a positive value indicates a 'better' score

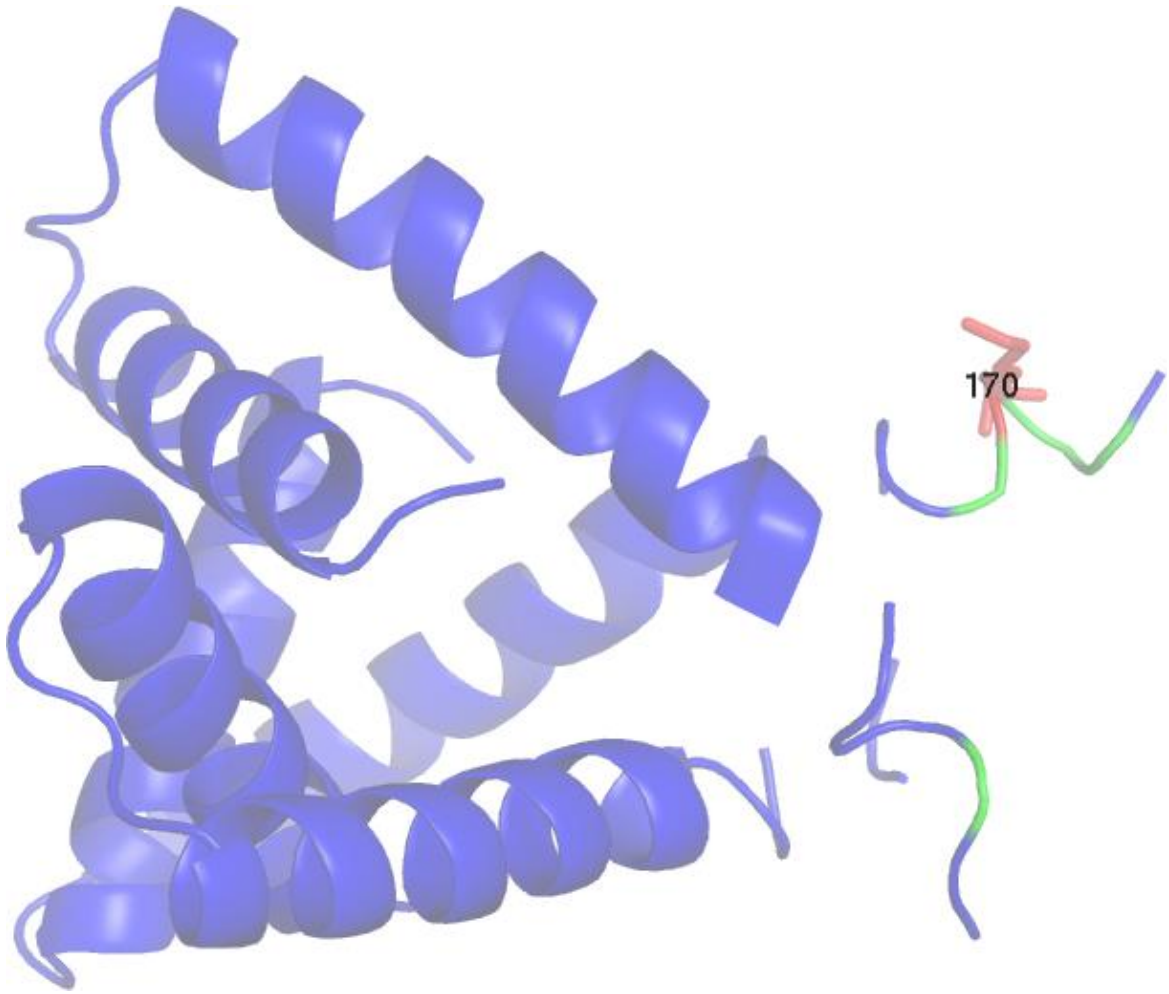



Procheck G-factor for all dihedral angles
G-factor
2
1
0
-1
-2
-3
-4
20
40
60
80
100
120
140
160
Residue number


Verify3D score over window of 7 residues
Verify3D score
1
0.5
0
-0.5
20
40
60
80
100
120
140
160
Residue number


Prosall (-ve) score over window of 7 residues
Prosall (-ve) score
6
4
2
0
-2
-4
20
40
60
80
100
120
140
160
Residue number


Residual VdW violations from MolProbity
violations
50
40
30
20
10
0
20
40
60
80
100
120
140
160
Residue number



Residue Plot of Ramachandran anlysis(based on data from Richardson Lab's Molprobity)

References:

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3. Sippl M J, "Recognition of Errors in Three-Dimensional Structures of Proteins", Proteins 17 (1993): 355-362
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5. Laskowski R Ai et al, "AQUA and PROCHECK_NMR: Programs for checking the quality of proteins structures solved by NMR", J Biomolec NMR 8 (1996): 477-486
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8. Word J M et al, "Asparagine and Glutamine: Using Hydrogen Atom Contacts in the Choice of Side-chain Amide Orientation", J Mol Biol 285 (1999): 1735-1747

9. Word J M et al, "Visualizing and Quantifying Molecular Goodness-of-Fit: Small-probe Contact Dots with Explicit Hydrogens", J Mol Biol 285 (1999): 1711-1733
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11. Luthy R, McLachlan A D and Eisenberg D, "Secondary Structure-Based Profiles: Use of Structure-Conserving Scoring Tables in Searching Protein Sequence Databases for Structural Similarities", Proteins 10 (1991): 229-239
12. Richardson D C, Richardson J S, "The kinemage: a tool for scientific communication", Prot Sci 1(1) (1992): 3-9
13. Koradi, R, et al, "MOLMOL: a program for display and analysis of macromolecular structures ", J Mol Graphics 14 (1996): 51-55.
14. Güntert, P, Mumenthaler, C & Wüthrich, K "Torsion angle dynamics for NMR structure calculation with the new program DYANA", J. Mol. Biol 273 (1997): 283-298
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Analysed by on May-10-2013 using PSVS 1.3

Software Environment

Software for structure quality evaluation:

```
DSSP            DsspCMBI-April-2000
pdbstat         PdbStat-5.4 Version
AutoAssign      Version 2.4.0 (uses only AVS scripts)
RPF analysis    ASDP-1.0
PDB validation  Version 8.061
Verify3D        Version 1.0 corrected by Aneerban
ProsaII         Prosa2003
PROCHECK        Version 3.5.4
MolMol          Version 2K.2
```

MolProbity programs:

```
cluster           1999
clashlistcluster  1999 (corrected by Aneerban)
```

```
mage              Version 6.35.040409
prekin            Version 6.35.040406
reduce            Version 2.14
probe             Version 2.6
```

Other Software:

```
PERL            Version 5.8.0
convert         ImageMagick 5.5.6
ps2pdf          Ghostscript 7.05
htmldoc         v1.9
gnuplot         Version 3.7 patchlevel 3
jpegtopnm       year 2000
pnmcrop         year 2000
pnmtojpeg       year 2000
```